

# Back-to-back emission of the electrons in double photoionization of helium

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## Abstract

We calculate the double differential distributions and distributions in recoil momenta for the high energy non-relativistic double photoionization of helium. We show that the results of recent experiments is the pioneering experimental manifestation of the quasifree mechanism for the double photoionization, predicted long ago in our papers. This mechanism provides a surplus in distribution over the recoil momenta at small values of the latter, corresponding to nearly "back-to-back" emission of the electrons. Also in agreement with previous analysis the surplus is due to the quadrupole terms of the photon-electron interaction. We present the characteristic angular distribution for the "back-to-back" electron emission. The confirmation of the quasifree mechanism opens a new area of exiting experiments, which are expected to increase our understanding of the electron dynamics and of the bound states structure. The results of this Letter along with the recent experiments open a new field for studies of two-electron ionization not only by photons but by other projectiles, e.g. by fast electrons or heavy ions.

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## I. INTRODUCTION

In this Letter we calculate the distribution in recoil momenta for the double photoionization of helium in the high energy nonrelativistic limit. We calculate also the energy distribution in the "back-to-back" configuration of the emitted electrons. Our calculations are in agreement with the results of recent experiments on the double ionization of helium by the photons with the energies 800 and 900 eV [1], [2], providing information on the distribution in recoil momenta  $q$  of the nucleus. Although the groups, which carried out the experiments [1], [2], did not present quantitative results, their experiments demonstrate that the distribution of outgoing electrons obtains a surplus at small  $q$  of about 2 a.u. The kinematics of these experiments enables to separate the non-dipole contributions at small values of  $q$ . Thus the observed surplus is entirely due to the non-dipole terms. The results of [1], [2] prove the existence of the *quasi-free mechanism* (QFM) of the double photoionization, which was predicted many years ago [3].

By that time only two mechanisms of the process were known. In both of them the electron, which interacted with the photon directly obtained almost all the incoming photon energy  $\omega$ . In the first, called *shake-off* the secondary electron was pushed to the continuum due to the sudden change of the effective field. In the second, called *knock-out* mechanism, the photoelectron inelastically collides with the bound one, sharing the photon energy. The two mechanisms could be clearly separated in the case of high photon energies

$$\omega \gg I, \tag{1}$$

with  $I$  standing for the single-particle binding energy, when the final state interactions between the outgoing electrons in the shake-off mechanism can be neglected.

The key point of the third mechanism, predicted in [3], is that the two electrons can absorb a photon almost without participation of the nucleus. This is impossible in the shake-off and knock-out mechanisms, since the single photoionization is not allowed for the free electrons and thus in ionization, caused by a photon carrying the energy  $\omega$ , momentum  $q = (2\omega)^{1/2}$  (in atomic system of units  $e = \hbar = m$ , adopted in this paper) should be transferred to the nucleus.

The QFM has several bright features. Before its prediction and decades after the common wisdom was that the photoelectrons energy spectrum curve has an **U** shape with high

maxima at the edge regions of the spectra. The QFM has predicted a local maximum at the center of the energy distribution leading to **W** shape. Another feature of QFM is that the contribution of it decreased with energy slower than the contributions of the other mechanisms. Thus, the account of QFM leads to the breakdown of the high energy non-relativistic asymptotic of the double-to single photoionization cross sections ratio. Also, the QFM requires going beyond the dipole approximation, since there is no dipole moment of the two-electron system at  $\mathbf{q} = 0$ ). One can see [4] for more details.

Although the paper [3] was cited rather often since its publication, QFM was for a long time not treated seriously by the physical community as a two-electron photoionization mechanism. For example, the QFM was not even mentioned in the review paper of Dalgarno and Sadeghpour [5]. Attempts were undertaken to check the QFM effects in purely computer calculations. These attempts fail to confirm the existence of the QFM. Later it was understood [8] that the QFM is extremely sensitive to the analytical properties of the initial state wave functions. In particular, it cannot be reproduced in computations with uncorrelated electron wavefunctions, which were used in the calculations, mentioned above.

Other developments were even more dramatic. Some of the calculations lead to the **W** shape of the spectrum (see, *e.g.* [6]) even in the dipole approximation. It was shown, however, in [9] that the central peak there was spurious, being entirely a consequence of oversimplified approximations for the wave functions of either initial or the final states. The consistent approach provided cancellation of spurious terms and restoration of the **U** shape of the spectrum in the dipole approximation.

## II. THE QUASIFREE MECHANISM

If the condition (1) is fulfilled, in the single photoionization process the momentum  $q$  exceeds strongly the characteristic binding momentum  $\eta$ . However, in the double photoionization there is a kinematical region, where the recoil momentum  $q$  can be as small as  $\eta$ . Following the general analysis of Bethe [7], one can expect the increasing of the differential cross section in this region. It happens because the bound electrons are localized mainly near their Bohr orbits with the radii  $r_b \sim 1/\eta$ . Each act of transferring larger momenta requires going to the smaller distances to the nucleus, where the electron density is smaller, leading to a smaller value of the amplitude.

In the rest frame of the initial atom the recoil momentum is

$$\mathbf{q} = \mathbf{k} - \mathbf{p}_1 - \mathbf{p}_2. \quad (2)$$

Here  $\mathbf{k}$  is the photon momentum,  $\mathbf{p}_i$  are the momenta of the outgoing electrons.

Except the edge region of the spectra both  $\varepsilon_i \gg I$ , and thus  $p_i \gg \eta$ . Hence, the QFM condition

$$\eta \leq q \ll p_{1,2}, \quad (3)$$

means that large momenta  $\mathbf{p}_i$  almost compensate each other. Hence, they are emitted mostly "back-to-back, with  $t \equiv (\mathbf{p}_1 \cdot \mathbf{p}_2)/p_1 p_2$  close to  $-1$ . The amplitude is large for  $|t + 1| \sim I/\omega \ll 1$ . The condition (3) can be satisfied if the difference between the energies of outgoing electrons  $\varepsilon_i$  is small enough:

$$\beta \equiv \frac{|\varepsilon_1 - \varepsilon_2|}{E} \leq \sqrt{\frac{2I}{E}}; \quad E = \varepsilon_1 + \varepsilon_2, \quad (4)$$

with  $E = \varepsilon_1 + \varepsilon_2$  the total energy carried by electrons.

As we have seen earlier, there is no dipole contribution in exactly free kinematics with  $q = 0$ . Such a process is caused by the quadrupole and higher multipole terms. In the quasifree kinematics there is a non-vanishing dipole term proportional to  $(\mathbf{eq})$ . However, it is strongly suppressed [8], and the quadrupole terms do dominate for  $\omega \geq 800$  eV. Anyway, in the experiment, described in [1] they detect the recoiling ions moving perpendicular to the polarization direction. This entirely eliminates the contribution of the dipole terms.

In the QFM the two bound electrons exchange large momenta in the initial state. Thus, they approach each other at small distances  $r_{12} < r_b$ , while their distances from the nucleus is still of the order of the Bohr orbit. Hence, it is reasonable to attribute the QFM amplitude to the properties of the initial state wave function  $\psi(r_1, r_2, r_{12})$  at  $r_{12} = 0$ . It was shown in [9] that the amplitude contains the factor  $\partial\psi/\partial r_{12}$  at  $r_{12} = 0$ , which is connected to the function

$$\phi(r) \equiv \psi(r, r, 0) \quad (5)$$

by the cusp condition [10].

### III. DISTRIBUTION IN RECOIL MOMENTA

Now let us calculate the QFM amplitude of the high energy nonrelativistic double photoionization.

Interactions of the outgoing electrons with the nucleus are determined by their Sommerfeld parameters  $\xi_i = Z/p_i$ . Since both  $\varepsilon_i \gg I$ , at the first step we can neglect interactions between the outgoing electrons and the nucleus [11]. Direct calculation provides

$$\frac{d^2\sigma}{dq^2 d\varepsilon_1} = \frac{128}{15} \frac{\omega}{cE^3} S^2(q^2), \quad (6)$$

with

$$S(q^2) = \int d^3r \phi(r) \exp(-i(\mathbf{q} \cdot \mathbf{r})), \quad (7)$$

with  $\phi(r)$  defined by Eq.(5).

The analytical expressions, approximating very precise wave functions [12] at  $r_{12} = 0$  were obtained in [13], [14]. These functions work as well for approximating the improved wave functions obtained in [15]. In the simplest case [13]

$$\phi(r) = \phi(0) \exp(-2Zr), \quad (8)$$

with  $Z$  being the charge of the nucleus. This provides

$$S(q^2) = \frac{16\pi Z \phi(0)}{(q^2 + 4Z^2)^2}. \quad (9)$$

For the functions obtained in [12, 15]  $\phi(0) \simeq 1.37$ . Thus indeed the distribution in recoil momentum  $q$  has a surplus at small  $q \ll p_i$ . To obtain the distribution  $d\sigma/dq^2$ , one should integrate the distribution (6) over  $\varepsilon_1$ , having in mind that  $q \geq |p_1 - p_2|$ . In actual calculations, instead of (8) we employ combination of two exponential terms [14] which gives a very accurate approximation of the exact wave function at the electron-electron coalescence line.

In the experiments [1, 2] the parameters  $\xi_i$  of the outgoing electrons are of the order 1/3. Thus, it is desirable to avoid expansion in  $\xi_i$ , taking into account interaction with the nucleus. In this case the factor  $\exp(-i(\mathbf{q} \cdot \mathbf{r}))$  in the integrand of Eq.(7) should be replaced by the product of the two continuum Coulomb functions. The integral can be evaluated analytically by employing the technique, developed in [16]. Finally we obtain

$$\frac{d^2\sigma}{dq^2 d\varepsilon_1} = \frac{128}{15} \frac{\omega}{cE^3} S^2(q^2) F(\xi_i, q^2). \quad (10)$$

The function  $F$  with  $F(\xi_1 = 0, \xi_2 = 0, q^2) = 1$  has a simple analytical form.

These equations enable to obtain the angular distribution at the point of exactly "back-to-back" emission by presenting

$$\frac{d^2\sigma}{dt d\varepsilon_1} = 2p_1 p_2 \frac{d^2\sigma}{dq^2 d\varepsilon_1}. \quad (11)$$

We calculate the distributions  $d^2\sigma/dtd\varepsilon_1$  and  $d\sigma/dt$  at the point of exactly "back-to-back" emission  $t = -1$ . In Fig.1 we provide example of the distribution  $d^2\sigma/dtd\varepsilon_1$  for the energy  $\omega=900$  eV employed in [2]. One can see that the main contribution to  $d\sigma/dt$  comes from  $\beta \leq 0.3$  in agreement with Eq.(4). In Fig 2. we show the dependence of the distribution  $d\sigma/dt$  on the photon energy in the region near 1 keV. At  $\omega=900$  eV we find  $d\sigma/dt = 0.52barn$ . Since the important interval of  $t$  is  $I/\omega \approx 0.06$  the contribution to the total cross section is  $0.03b$  in agreement with [17].

#### IV. SUMMARY

We have calculated the distributions  $d^2\sigma/dq^2d\varepsilon_1$  and  $d\sigma/dq^2$  for the non-relativistic high energy double photoionization. Our results are consistent with those of the recent experiments [1], [2]. Distribution in recoil momentum  $q$  has a surplus at small  $q$  caused by the quadrupole terms of electron-photon interaction. Thus, the existence of quasifree mechanism predicted long ago [3] is confirmed. This opens a new area for experimental investigations of this mechanism. Note that the relative role of the QFM grows with the photon energy increase, and its manifestation for  $\omega$  beyond the keV region is expected to be even more prominent. It is expected that the corresponding experimental and theoretical investigations will add much to our knowledge of the electron dynamics in the process of two-electron ionization and of the structure of the bound states wave functions.

We dream that further research will move into relativistic region  $\omega \geq c^2$  thus disclosing the fine structure of the central peak of the energy distribution, caused by the non-dipole nature of the QFM. We hope also that contribution of the QFM to the total cross section, resulting in a slope of the double-to-single photoionization ratio will be measured. We expect the detailed investigation of the really relativistic case, where the QFM contribution should become as important as that of the shake-off and even much overcome it.

Also, investigation of the QFM enables to clarify behavior of the wave function of the atom of helium near the singular electron-electron coalescence point. Besides the purely theoretical interest, this is important for precise computations of the atomic characteristics. Recall that the proper treatment of the three-particle coalescence point enabled to diminish strongly the number of parameters in the bound state wave functions.

We expect that the results, presented in this Letter along with the recent experiments

will stimulate studies of two-electron ionization by the other types of projectiles, such as the fast electrons or heavy ions, where along with quadrupole, monopole terms will contribute at least not less.

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FIG. 1: Energy distribution for the "back-to-back" emission ( $t = -1$ ) presented by Eq.(11) for  $\omega = 900eV$  considered in [2]. The value  $d^2\sigma/d\varepsilon_1 dt$  is given in *barn/eV*.

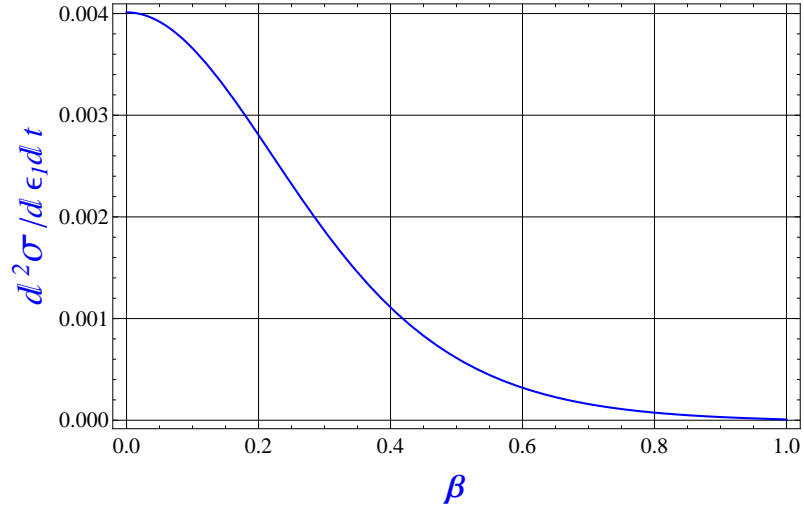




FIG. 2: Dependence of the differential distribution  $d\sigma/dt$  at  $t = -1$  on the photon energy in keV region. The value of  $d\sigma/dt$  is given in barns.

